provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JUN 2010 HIGHEST RN 1227141-97-0
DICTIONARY FILE UPDATES: 7 JUN 2010 HIGHEST RN 1227141-97-0

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TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html
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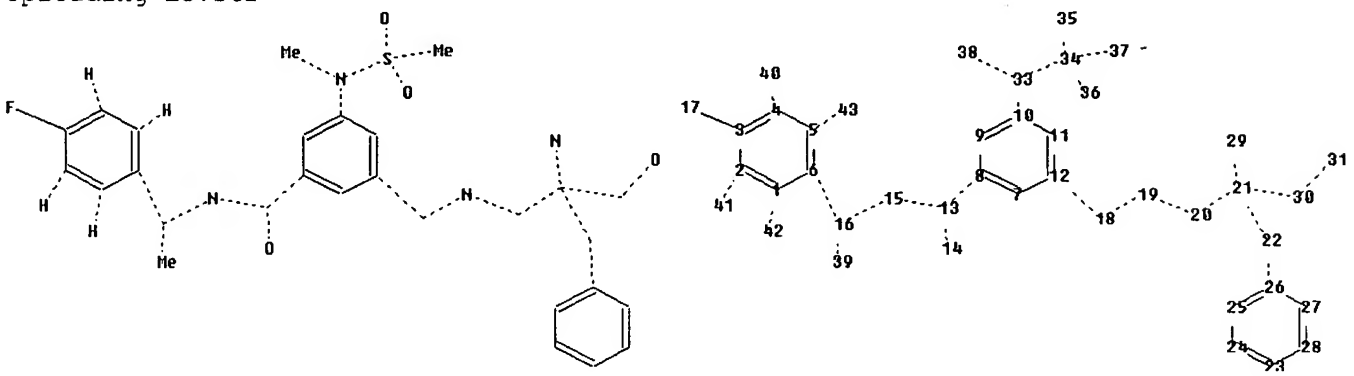

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ring nodes :
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chain bonds :
1-42 2-41 3-17 4-40 5-43 6-16 8-13 10-33 12-18 13-14 13-15 15-16 16-39 18-19 19-20 20-21 21-22 21-29 21-30 22-26 30-31 33-34 33-38 34-35 34-36 34-37
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
1-42 2-41 4-40 5-43 6-16 8-13 10-33 12-18 13-14 13-15 15-16 16-39 18-19 19-20 20-21 21-22 21-29 21-30 22-26 30-31 33-34 33-38 34-35 34-36 34-37
exact bonds :
3-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 23-24 23-28 24-25 25-26 26-27 27-28

Connectivity :
13:3 E exact RC ring/chain 14:1 E exact RC ring/chain 15:2 E exact RC ring/chain 18:2 E exact RC ring/chain 19:2 E exact RC ring/chain 20:2 E exact RC ring/chain

22:2 E exact
RC ring/chain 29:1 E exact RC ring/chain 30:2 E exact RC ring/chain 31:1 E exact RC ring/chain

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
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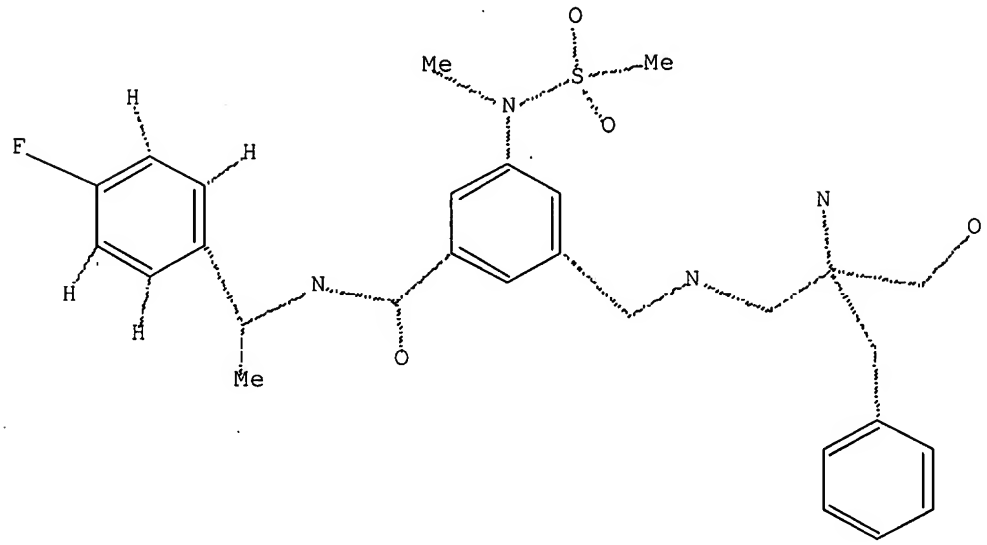

Structure attributes must be viewed using STN Express query preparation.
L5 3 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 950 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 11:28:27 ON 08 JUN 2010
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FILE COVERS 1907 - 8 Jun 2010 VOL 152 ISS 24
FILE LAST UPDATED: 7 Jun 2010 (20100607/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L6
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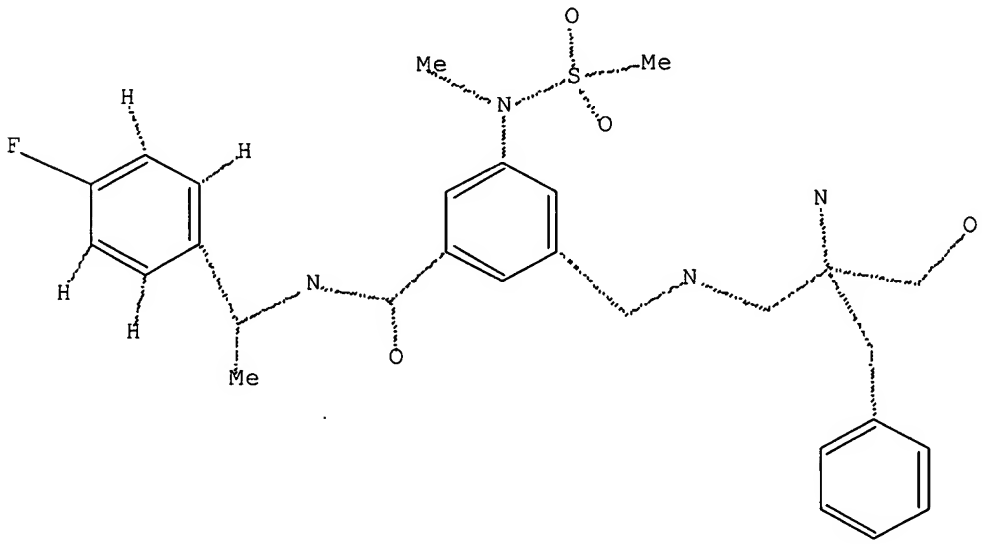

Structure attributes must be viewed using STN Express query preparation.
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L6 2 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L5

=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 11:28:41 ON 08 JUN 2010
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FILE LAST UPDATED ON November 14, 2009

FILE COVERS 1779 TO 2009.
*** FILE CONTAINS 10,654,725 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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http://www.stn-international.com/stn_chemistry_beilstein.html

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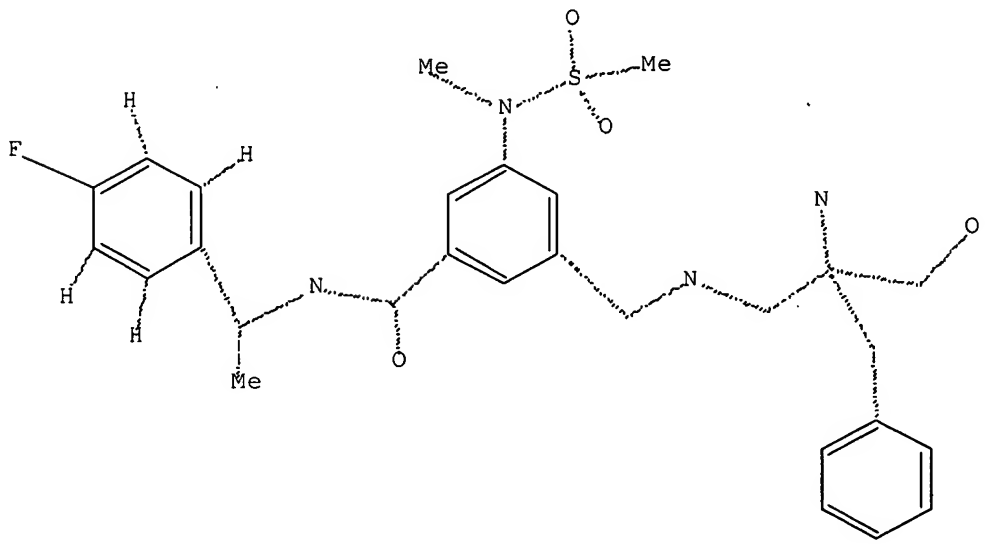

Structure attributes must be viewed using STN Express query preparation.
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100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

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FILE LAST UPDATED:          4 JUN 2010   <20100604/UP>
MOST RECENT UPDATE:           201035      <201035/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
>>> Now containing more than 1.5 million chemical structures in DCR <<<

>>> IPC, ECLA, US National Classifications and Japanese F-Terms
    and FI-Terms have been updated with reclassifications to
    end of March 2010.
    No update date (UP) has been created for the reclassified
    documents, but they can be identified by
    specific update codes (see HELP CLA for details) <<<

>>> FOR THE LATEST DERWENT WORLD PATENTS INDEX (DWPI)
    STN USER DOCUMENTATION, PLEASE VISIT:
    http://www.stn-international.com/stn_dwpi.html <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> For changes in DWPI see HELP CHANGE - last updated April 6, 2010 <<<

>>> New display format ALLSTR available - see NEWS  <<<

>>> US National Patent Classification thesaurus added - see NEWS <<<
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

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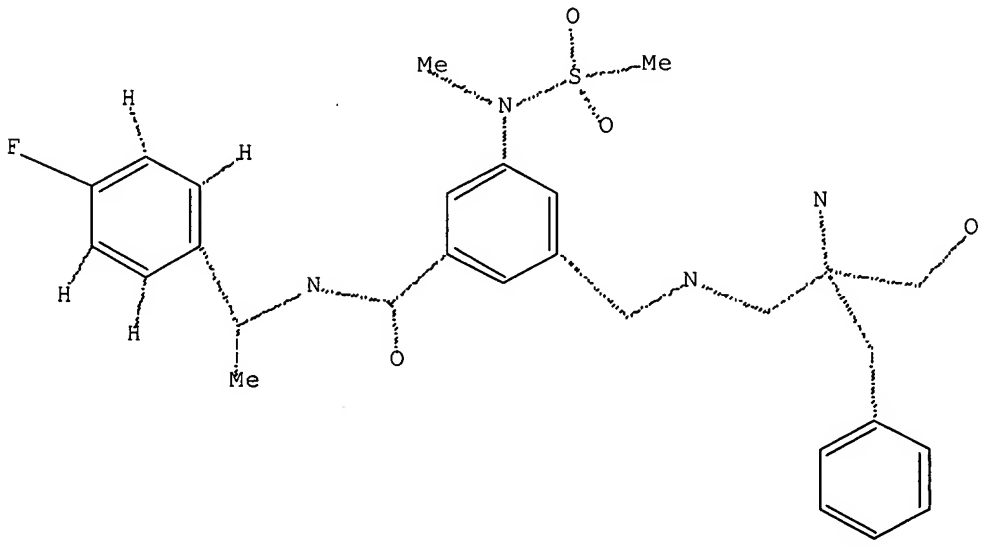


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PROCESSING COMPLETED FOR L6
PROCESSING COMPLETED FOR L11
L12             2 DUP REM L6 L11 (1 DUPLICATE REMOVED)
                  ANSWERS '1-2' FROM FILE ZCAPLUS

=> d ibib abs hitstr L12 1-2

L12  ANSWER 1 OF 2  ZCAPLUS  COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:324002  ZCAPLUS  Full-text
DOCUMENT NUMBER:          142:373552
TITLE:                    Benzyl ethers and benzylamines as beta-secretase
                          inhibitors, their preparation and use for the
                          treatment of Alzheimer's disease
INVENTOR(S):              Nantermet, Philippe G.; Rajapakse, Hemaka Anthony;
                          Selnick, Harold G.
PATENT ASSIGNEE(S):       Merck & Co., Inc., USA
SOURCE:                   PCT Int. Appl., 47 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     WO 2005032471         A2    20050414    WO 2004-US32009         20040929
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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     AU 2004277981         B2    20091001
     CA 2540452            A1    20050414    CA 2004-2540452         20040929
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     CN 1859904            A     20061108    CN 2004-80028599        20040929
     JP 2007507515         T     20070329    JP 2006-534062          20040929
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US 20060293380 A1 20061228 US 2006-573232 20060323
PRIORITY APPLN. INFO.: US 2003-508369P P 20031003
WO 2004-US32009 W 20040929
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 142:373552
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a group of benzyl ethers and benzylamines I which are inhibitors of the beta-secretase enzyme. In compds. I, X is O or NH; Y is CH or N; R1 is selected from aryl, arylmethyl, heterocyclyl, and heterocyclylmethyl, wherein the ring is unsubstituted or substituted with one or more substituents selected from halo, OH, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, cyano, and C1-6 alkoxy; R2 is selected from alkyl(alkylsulfonyl)amino, (alkylsulfonyl)amino, o-cyanophenyl, and, gem-cyanocycloalkyl; R3 is selected from (un)substituted (arylalkyl)aminocarbonyl, aminocarbonyl, alkylaminocarbonyl, cyclopropylethenyl, cyclopropylmethyloxy, and cyclopropylmethylamino; and includes all pharmaceutically acceptable salts. The invention also relates to the preparation of I, pharmaceutical compns. comprising these compds. and a pharmaceutically acceptable carrier, and the use of these compds. and compns. in the treatment of diseases in which the beta-secretase enzyme is involved, such as Alzheimer's disease. N-Methylsulfonylation of di-Me 5-aminoisophthalate, followed by N-methylation, gave II, which was partially hydrolyzed and coupled with a chiral amine to give III. Hydrolysis of III followed by borane reduction, bromination, and substitution with 2-amino-2-benzylpropane-1,3-diol, prepared by reduction of racemic α-benzylserine, resulted in the formation of IV. The compds. of the invention inhibit the beta-secretase enzyme, generally with IC50 values from about 1 nM to 100 μM.

IT **849623-02-5P**, 3-[[(2-Amino-2-benzyl-3-hydroxypropyl)amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]benzamide trifluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzyl ethers and benzylamines as beta-secretase inhibitors for the treatment of Alzheimer's disease)

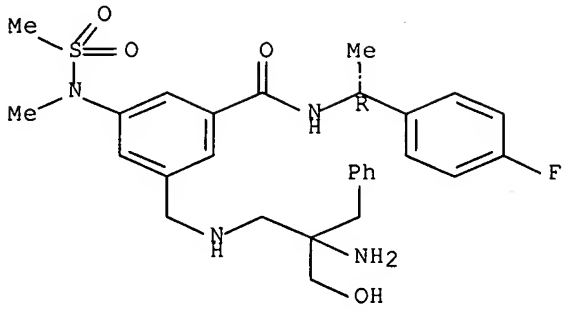
RN 849623-02-5 ZCAPLUS

CN Benzamide, 3-[[[2-amino-2-(hydroxymethyl)-3-phenylpropyl]amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 849623-01-4
CMF C28 H35 F N4 O4 S

Absolute stereochemistry.



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CRN 76-05-1
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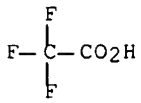


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 2 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2010:295671 ZCAPLUS Full-text
DOCUMENT NUMBER: 152:516542
TITLE: SAR of tertiary carbinamine derived BACE1 inhibitors: Role of aspartate ligand amine pK a in enzyme inhibition
AUTHOR(S): Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Barrow, James C.; McGaughey, Georgia B.; Munshi, Sanjeev; Lindsley, Stacey R.; Young, Mary Beth; Ngo, Phung L.; Katherine Holloway, M.; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel; Vacca, Joseph P.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2010), 20(6), 1885-1889
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The optimization of tertiary carbinamine derived inhibitors of BACE1 from its discovery as an unstable lead to low nanomolar cell active compds. is

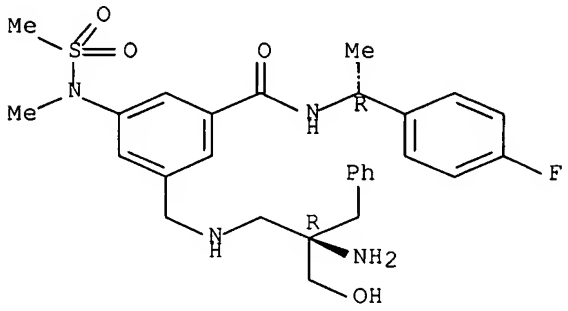
described. Five-membered heterocycles are reported as stable and potency enhancing linkers. In the course of this work, we have discovered a clear trend where the activity of inhibitors at a given assay pH is dependent on pK a of the amino group that interacts directly with the catalytic aspartates. The potency of compds. as inhibitors of Aβ production in a cell culture assay correlated much better with BACE1 enzyme potency measured at pH 7.5 than at pH 4.5.

IT 1225027-40-6
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tertiary carbinamine-derived BACE1 inhibitors preparation and role of aspartate ligand amine pK a in enzyme inhibition)

RN 1225027-40-6 ZCAPLUS

CN Benzamide, 3-[[[(2R)-2-amino-2-(hydroxymethyl)-3-phenylpropyl]amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3             STRUCTURE UPLOADED
L4           0 SEA SSS SAM L3
L5           3 SEA SSS FUL L3
               D SCA

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L6           2 SEA SPE=ON  ABB=ON  PLU=ON  L5

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L7           0 SEA SSS SAM L3
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L9           0 SEA SSS SAM L3
L10          1 SEA SSS FUL L3
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               D STAT QUE L8

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               D STAT QUE L11

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L12          2 DUP REM L6 L11 (1 DUPLICATE REMOVED)
                    ANSWERS '1-2' FROM FILE ZCAPLUS
               D IBIB ABS HITSTR L12 1-2


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
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     STRUCTURE FILE UPDATES:     7 JUN 2010  HIGHEST RN 1227141-97-0
     DICTIONARY FILE UPDATES:    7 JUN 2010  HIGHEST RN 1227141-97-0

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     TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

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FILE ZCAPLUS

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FILE COVERS 1907 - 8 Jun 2010 VOL 152 ISS 24
FILE LAST UPDATED: 7 Jun 2010 (20100607/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON November 14, 2009

FILE COVERS 1779 TO 2009.
FILE CONTAINS 10,654,725 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *

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      * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                    *
      * FOR PRICE INFORMATION SEE HELP COST                             *
      ******************************************************************

      >>> FOR THE LATEST BEILSTEIN STN USER DOCUMENTATION, PLEASE VISIT:
          http://www.stn-international.com/stn_chemistry_beilstein.html


      FILE WPIX
      FILE LAST UPDATED:          4 JUN 2010   <20100604/UP>
      MOST RECENT UPDATE:           201035      <201035/DW>
      DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
      >>> Now containing more than 1.5 million chemical structures in DCR <<<

      >>> IPC, ECLA, US National Classifications and Japanese F-Terms
          and FI-Terms have been updated with reclassifications to
          end of March 2010.
          No update date (UP) has been created for the reclassified
          documents, but they can be identified by
          specific update codes (see HELP CLA for details) <<<

      >>> FOR THE LATEST DERWENT WORLD PATENTS INDEX (DWPI)
          STN USER DOCUMENTATION, PLEASE VISIT:
          http://www.stn-international.com/stn_dwpi.html <<<

      >>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

      >>> For changes in DWPI see HELP CHANGE - last updated April 6, 2010 <<<

      >>> New display format ALLSTR available - see NEWS  <<<

      >>> US National Patent Classification thesaurus added - see NEWS <<<

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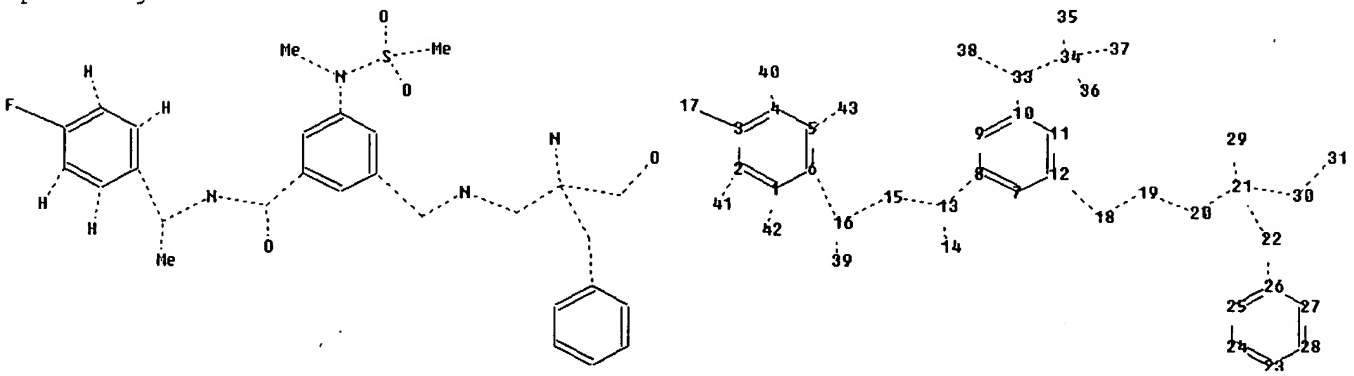

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41  42  43
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  23  24  25  26  27  28
chain bonds :
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34-37
ring bonds :
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```

```
25
25-26  26-27  27-28
exact/norm bonds :
1-42  2-41  4-40  5-43  6-16  8-13  10-33  12-18  13-14  13-15  15-16  16-39  18-19
19-20  20-21  21-22  21-29  21-30  22-26  30-31  33-34  33-38  34-35  34-36  34-37
exact bonds :
3-17
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12  23-24  23-28  24-
25
25-26  26-27  27-28


Connectivity :
13:3 E exact RC ring/chain  14:1 E exact RC ring/chain  15:2 E exact RC ring/chain
18:2 E exact RC ring/chain  19:2 E exact RC ring/chain  20:2 E exact RC ring/chain
22:2 E exact
RC ring/chain  29:1 E exact RC ring/chain  30:2 E exact RC ring/chain  31:1 E exact
RC ring/chain

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:CLASS  20:CLASS  21:CLASS
22:CLASS  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:CLASS  30:CLASS
31:CLASS
33:CLASS  34:CLASS  35:CLASS  36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS
41:CLASS  42:CLASS
43:CLASS
```